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NEWS 16 JAN 02 STN pricing information for 2008 now available  
NEWS 17 JAN 16 CAS patent coverage enhanced to include exemplified  
prophetic substances  
NEWS 18 JAN 28 USPATFULL, USPAT2, and USPATOLD enhanced with new  
custom IPC display formats  
NEWS 19 JAN 28 MARPAT searching enhanced  
NEWS 20 JAN 28 USGENE now provides USPTO sequence data within 3 days  
of publication  
NEWS 21 JAN 28 TOXCENTER enhanced with reloaded MEDLINE segment  
NEWS 22 JAN 28 MEDLINE and LMEEDLINE reloaded with enhancements  
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NEWS 24 FEB 20 PCI now available as a replacement to DPCI  
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U.S. National Patent Classification  
NEWS 28 MAR 31 IFICDB, IFIPAT, and IFIUDB enhanced with new custom  
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spectra  
NEWS 30 MAR 31 CA/Caplus and CASREACT patent number format for U.S.  
applications updated  
NEWS 31 MAR 31 LPCI now available as a replacement to LDPCI  
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NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,  
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|                      |            |         |
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| => file casreact     |            |         |
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL   |
|                      | ENTRY      | SESSION |
| FULL ESTIMATED COST  | 0.42       | 0.42    |

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FILE CONTENT:1840 - 29 Mar 2008 VOL 148 ISS 14

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\*\*\*\*\*  
\* \* \* \* \*  
\* CASREACT now has more than 13.8 million reactions \*  
\* \* \* \* \*  
\*\*\*\*\*

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Program Files\Stnexp\Queries\10553993-first-rejection.str

L1      STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1      STR

===== I—I —————> ————— I

Structure attributes must be viewed using STN Express query preparation.

=> s l1  
SAMPLE SEARCH INITIATED 13:50:52 FILE 'CASREACT'  
SCREENING COMPLETE - 646 REACTIONS TO VERIFY FROM 115 DOCUMENTS

100.0% DONE 646 VERIFIED 307 HIT RXNS 50 DOCS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 11396 TO 14444  
PROJECTED ANSWERS: 850 TO 1830

L2 50 SEA SSS SAM L1 ( 307 REACTIONS)

=> s l1 full  
FULL SEARCH INITIATED 13:50:58 FILE 'CASREACT'  
SCREENING COMPLETE - 13218 REACTIONS TO VERIFY FROM 2023 DOCUMENTS

100.0% DONE 13218 VERIFIED 7572 HIT RXNS 1237 DOCS  
SEARCH TIME: 00.00.05

L3 1237 SEA SSS FUL L1 ( 7572 REACTIONS)

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 118.42 118.84

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FILE COVERS 1907 - 2 Apr 2008 VOL 148 ISS 14  
FILE LAST UPDATED: 1 Apr 2008 (20080401/ED)

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=> s l3  
L4 1237 L3

=> s l3 and free radical  
1237 L3  
1368029 FREE  
328527 RADICAL  
74182 FREE RADICAL

(FREE(W) RADICAL)  
 L5 13 L3 AND FREE RADICAL  
 => s 13 and radical  
 1237 L3  
 328527 RADICAL  
 L6 98 L3 AND RADICAL  
 => s 13 and initiator  
 1237 L3  
 74166 INITIATOR  
 L7 4 L3 AND INITIATOR  
 => s peroxide? or diazo? or dialkylphenylalkane?  
 247525 PEROXIDE?  
 112472 DIAZO?  
 0 DIALKYLPHENYLALKANE?  
 L8 359023 PEROXIDE? OR DIAZO? OR DIALKYLPHENYLALKANE?  
 => s 18 and 13  
 1237 L3  
 L9 28 L8 AND L3  
 => s 19 and 16  
 L10 4 L9 AND L6  
 => s 17 or 110  
 L11 8 L7 OR L10  
 => s 111 not py > 2003  
 5547651 PY > 2003  
 L12 6 L11 NOT PY > 2003  
 => d 112 ibib abs hitstr 1-  
 YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

L12 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on SIN  
 ACCESSION NUMBER: 2001:228100 CAPLUS  
 DOCUMENT NUMBER: 135:92680  
 TITLE: Iodine atom transfer addition reaction of 1-iodoalkyl  
 phosphonates to alkenes in the presence of  
 $\alpha,\alpha'$ -azoisobutyronitrile (AIBN):  
 mechanistic aspects  
 AUTHOR(S): Balczewski, Piotr; Mikolajczyk, Marian  
 CORPORATE SOURCE: Centre of Molecular and Macromolecular Studies, Polish  
 Academy of Sciences, Lodz, 90-363, Pol.  
 SOURCE: New Journal of Chemistry (2001), 25(4), 659-663  
 CODEN: NJCHE5; ISSN: 1144-0546  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:92680  
 AB The mechanistic pathway of the title reaction, which constitutes the 1st  
 example of a radical I atom transfer addition reaction of  
 nonfluorine-containing  
 phosphonates, will determine whether 2-iodo-2-methylpropionitrile, 8, can serve  
 as a competing I donor with the starting di-Et 1-iodoalkyl phosphonates,  
 1a,b. The title reaction proceeds with AIBN as the sole radical  
 initiator, not requiring poisonous Sn reagents as co-initiators,  
 and gave di-Et 3-iodoalkylphosphonates 3a-e (the final products of the  
 propagation step, isolated in 59-95% yield), tetramethylsuccinodinitrile,  
 9, di-Et methylphosphonate, 4, and tetra-Et ethylenebisphosphonate 5 (all  
 termination products, 0-10% yields). The radical character of this

reaction was demonstrated using TEMPO as a radical trap. 8 (the intermediate of the initiation step), synthesized independently from AIBN and I, caused complete inhibition of the reaction when added to the reaction mixture, indicating that it does not behave as an I donor in the transfer stage, but rather as an inhibitor.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:656498 CAPLUS

DOCUMENT NUMBER: 125:328880

TITLE: The Synthesis of Phosphonate Ester Containing Fluorinated Vinyl Ethers

AUTHOR(S): Pedersen, Scot D.; Qiu, Weiming; Qiu, Zai-Ming; Kotov, Stefan V.; Burton, Donald J.

CORPORATE SOURCE: Department of Chemistry, University of Iowa, Iowa City, IA, 52242, USA

SOURCE: Journal of Organic Chemistry (1996), 61(23), 8024-8031  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:328880

AB Three novel perfluorovinyl ethers containing phosphonate ester groups, di-Et 1,1,2,2,3,3,5,6,6-nonafluoro-4-oxa-5-hexenylphosphonate, (EtO)2P(O)(CF2)3OCF2CF2 (1), di-Et 1,1,2,2,4,4,5,5-heptafluoro-3-oxa-4-pentenylphosphonate, (EtO)2P(O)(CF2)2OCF2CF2 (2), and di-Et 1,1,2,2,4,4,5,5,7,8,8-decafluoro-4-trifluoromethyl-3,6-dioxo-7-octenylphosphonate, CF2(CFOCF2CF(CF3)O(CF2)2P(O)(OEt)2 (3), have been synthesized. Perfluoro vinyl ethers 1 and 2 were synthesized from Me 4-trifluoroethenoxy-2,2,3,3,4,4-hexafluorobutanoate and Me 3-trifluoroethenoxy-2,2,3,3-tetrafluoropropanoate, resp., while perfluorovinyl ether 3 was synthesized either from 5-trifluoroethenoxy-4-trifluoromethyl-3-oxa-1,1,2,2,4,4,5,5-heptafluoropentylsulfonyl fluoride or Me 6-trifluoroethenoxy-5-trifluoromethyl-4-oxa-2,2,3,3,5,6,6-heptafluorohexanoate. The carboxylate esters were converted to the corresponding fluoroalkyl iodides via a free-radical iododecarboxylation. The sulfonyl fluoride was converted to its corresponding fluoroalkyl iodide via iododesulfination. The intermediate iodides were useful precursors for the incorporation of the phosphonic ester groups via a photoreaction with tetra-Et pyrophosphite to produce di-Et fluorophosphonites. The di-Et fluorophosphonites were oxidized to the desired phosphonates, 1, 2, and 3, utilizing hydrogen peroxide as the oxidant. Moderate to good overall yields of perfluorovinyl ethers 1-3 have been achieved.

L12 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:255278 CAPLUS

DOCUMENT NUMBER: 118:255278

TITLE: Stereocontrolled construction of substituted pyrrolidines based on intramolecular protodesilylation reaction. Enantiospecific synthesis of (-)-kainic acid and (+)-allokainic acid from L-serine

AUTHOR(S): Hatakeyama, Susumi; Sugawara, Kazutoshi; Takano, Seiichi

CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan

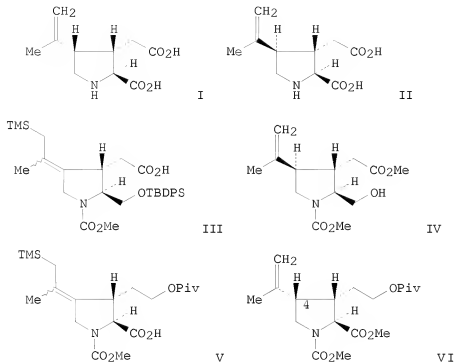
SOURCE: Journal of the Chemical Society, Chemical Communications (1993), (2), 125-7  
CODEN: JCCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:255278

GI



AB Novel stereocontrolled enantiospecific syntheses of (-)-kainic acid (I) and (+)-allokainic acid (II) have been achieved starting from L-serine via two modes of C-2 and C-3 side chain-directed intramol. protodesilylations of 4-(trimethylsilylmethyl)ethylidenepyrrolidines. Thus, the BF<sub>3</sub>.Et<sub>2</sub>O-mediated intramol. protodesilylation reaction of silylated pyrrolidine derivative III (TMS = trimethylsilyl, TBDPS = tert-butyl-diphenylsilyl) followed by methylation with CH<sub>3</sub>N and HF cleavage gave 3,4-trans-pyrrolidine IV with complete diastereoselectivity. IV was converted to II in 3 steps. On the other hand, the BF<sub>3</sub>.Et<sub>2</sub>O-mediated intramol. protodesilylation reaction of silylated pyrrolidine derivative V under diluted conditions proceeded with opposite diastereoselectivity to give 3,4-cis-pyrrolidine VI and its C-4 epimer in a ratio of 5.3:1. VI was converted to I.

L12 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 1990:7316 CAPLUS

DOCUMENT NUMBER: 112:7316

TITLE: Stereoselective exocyclic double-bond formation via

vinyl-radical cyclization

AUTHOR(S): Munt, Simon P.; Thomas, Eric J.

CORPORATE SOURCE: Dyson Perrins Lab., Oxford, OX1 3QY, UK

SOURCE: Journal of the Chemical Society, Chemical

Communications (1989), (8), 480-2

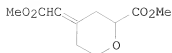
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 112:7316

GI



I

AB A stereoselective route to 2,6-cis-disubstituted 4-methoxycarbonylmethylenetetrahydropyrans, e.g., I, has been developed which uses a vinyl radical cyclization to establish the geometry of the exocyclic double bond, e.g., of  $\text{MeO}_2\text{CCH}=\text{CRCH}_2\text{CH}_2\text{OC}(\text{:CH}_2)\text{CO}_2\text{Me}$  (R = Br, iodo).

L12 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:166291 CAPLUS

DOCUMENT NUMBER: 102:166291

ORIGINAL REFERENCE NO.: 102:26137a,26140a

TITLE: Exchange of bromine and chlorine by iodine in haloaliphatic compounds induced by pentacarbonyliron

AUTHOR(S): Amriev, R. A.; Velichko, F. K.; Freidlina, R. Kh.

CORPORATE SOURCE: Inst. Elementoorg. Soedin., Moscow, USSR

SOURCE: Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1985), (1), 226-8

CODEN: IASKA6; ISSN: 0002-3353

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 102:166291

AB  $\text{Fe}(\text{CO})_5$  initiated the exchange reactions of RX (R = pentyl, Bu, allyl; X = Cl, Br) with I<sub>2</sub> or CHI<sub>3</sub> to give RI.

L12 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:45503 CAPLUS

DOCUMENT NUMBER: 102:45503

ORIGINAL REFERENCE NO.: 102:7145a,7148a

TITLE: Intramolecular Simmons-Smith reaction and other synthetic alternatives to cyclopropanation of dienic diazo ketones. Parallel decomposition pathways of a sterically congested diazo ketone and its vinylcyclopropane under thermal, photolytic, acid-catalyzed, and radical-release conditions

AUTHOR(S): Hudlicky, Tomas; Ranu, Brindaban C.; Naqvi, Saiyid M.; Srnak, Ana

CORPORATE SOURCE: Dep. Chem., Virginia Polytechnic Inst. and State Univ., Blacksburg, VA, 24061, USA

SOURCE: Journal of Organic Chemistry (1985), 50(1), 123-7

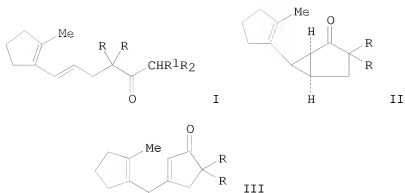
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:45503

GI



AB The decomposition of the diazo dienones I ( $R = H, Me$ ;  $R_1R_2 = :N_2$ ) under thermal, photolytic, and acid catalyzed conditions was examined. I ( $R = Me$ ,  $R_1R_2 = :N_2$ ) was converted into geminal dihalides I ( $R_1, R_2 = Br, iodo$ ), which were decomposed under conditions necessitating radical formation. The products, which were mostly the same, of these expts. included the cyclopropane II and the enone III. Reasons for the parallel outcomes of the expts. were discussed.